



# Theoretical prediction of temperature dependent shear modulus of bulk metallic glasses



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## ABSTRACT

A model of temperature dependent shear modulus and Young's modulus in bulk metallic glasses is established. The inherent relationship between the glass transition temperatures, the Debye temperature and shear modulus of bulk metallic glasses is revealed. The temperature dependent shear modulus can be predicted by our model without any fitting parameter. The model is presented based on a critical energy density criterion for plastic yielding which is derived from fundamental thermodynamics. This critical energy density consists of two parts: the heat added to the system and the input of mechanical energy, which are not completely equivalent. The agreement between theoretical results and experimental results is striking. And it is found that the temperature dependent Young's modulus could also be predicted pretty well by our model.

## 1. Introduction

Owing to the absence of defects such as dislocations and grain boundaries, the bulk metallic glasses (BMGs) have been reported to possess ultrahigh strength, high toughness and high wear resistance. There has been a substantial interest in the superior mechanical properties of BMGs in the past few decades. A lot of effort has been devoted to reveal the primary deformation units and clarify yielding behavior as well as the deformation mechanisms in BMGs [1–5]. The deformation and flow properties of BMGs are well described by the shear models with the result that shear modulus is expected to yield important information about their mechanical properties [6,7]. General metal materials become very brittle at low temperature, but BMGs still have excellent performance. Special types of metallic glasses are being developed for space exploration, which has excellent wear resistance, high strength, and can be used at extremely low temperature. Thus, the understanding of how temperature affects the mechanical properties of amorphous structure is, therefore, of considerable interest to the future design of BMGs with desired mechanical properties.

The temperature dependence of elastic moduli has been studied for a long time. Recently innovative experimental technologies are being actively developed for the temperature dependence of elastic moduli [8–10]. But the early classical phenomenological models continue to be used [11,12], which contain more or less fitting parameters. Although there are some new theoretical methods to predict the temperature dependence of elastic moduli of crystalline materials [13–16]. The

elastic properties of amorphous substance are relatively less understood. In the past few years, many significant research efforts have been also devoted to the study of the elastic moduli of BMGs [17–22]. Wang et al. found that there is a close link between the molar volume (or micro-structure) and elastic moduli of BMGs [19]. Wu et al. established a universal and simple correlation between the shear modulus and the specific length scale  $\lambda$  (wave length) [20]. These relationships are a very interesting and meaningful conclusion, which can be used to predict the shear modulus of BMGs at a certain temperature. Based on the Varshni equation which has two fitting parameters, Zhang et al. developed an effective method to simulate the temperature dependence of the shear modulus of BMGs by supposing that one fitting parameter is equal to the Debye temperature [21]. Lu et al. modified Zhang's model, and a good agreement between the calculated results and experimental data was reached for the temperature dependence of the shear modulus [22]. Temperature dependences of elastic moduli for representative BMGs are in situ studied down to liquid nitrogen temperature by Yu et al. [23]. It can be concluded that the elastic moduli of BMGs have been extensively studied. However, a physical description of the correlation between elastic moduli and temperature has not been established quantitatively without any fitting parameter. Therefore, it is necessary to reveal the law of elastic moduli's temperature dependence.

## 2. Model

Since no defects such as dislocations or grain boundaries exist, the

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elastic moduli of BMGs have long been considered to be closely related to the physical parameters determined by atomic cohesive energy, such as their component elements, glass transition temperatures ( $T_g$ ) and thermal expansion coefficients. On the basis of atomistic simulations and sheared bubble raft experiments, a shear transformation zone (STZ) model was introduced to explain the plastic deformation of metallic glasses [24,25]. According to this model, shear deformation takes place by spontaneous and cooperative reorganization of a small cluster of randomly close-packed atoms (localized shearing) [26]. The shear deformation of STZ under low temperature can be visualized as sliding between two thin disks of layer atoms around a free volume site which is achieved by the atom jumping [27]. And local shear deformations are due to the sharp increase of the atom mobility and softening along a shear plane motivated by the input of mechanical energy [28,29]. According to literature, the fracture will occur when the energy over the shear plane arisen from the elastic strain energy applied during the loading process, and that the total energy determines when the glassy specimen starts the localized shearing [30,31]. In Bron's theory, the temperature dependence of the elastic constants arises from the variation of the lattice potential energy [32].

As discussed above, it can be concluded that both thermal energy and mechanical energy contribute to overcoming the bonding force between atoms. So an assumption is proposed that there is a maximum critical energy density which is corresponding to the onset of the plastic yielding of shear bands. This critical energy density consists of two parts: the heat added to the system and the input of mechanical energy. Although the strain energy upon loading can transfer to heat during shear deformation. The strain energy is used to determine the starting of localized shearing in this work. Thus, the heat transferred from strain energy because of shear deformation or plastic deformation can be ignored. It is well known that the thermal activated atomic jumps do not cause shear strain, but the atoms move toward the shear direction under applied shear stress [33]. Thus, the heat added to the system and the input of mechanical energy are not completely equivalent. Based on the points discussed above, the critical energy density can be expressed as follows

$$E_{\text{cri}} = (W + \kappa Q)/V_s, \quad (1)$$

where  $E_{\text{cri}}$  is the critical energy density,  $W$  is the work done to the system,  $Q$  is the increase of internal energy due to temperature increasing from 0 K, and  $\kappa$  is an effective coefficient characterizing to what degree the internal energy contribute to shearing,  $V_s$  is the volume which undergoes local shearing which is the product of area and thickness for shear band. The formation of shear bands is dominated by shear deformation, so this process can be considered to be isastic. According to recent experimental studies and numerical simulations, the yielding of BMGs corresponds to the unstable propagation of a large number of local shearing events with a critical shear strain [26,34]. Hence, the input of mechanical energy can be written as

$$W = V_s \gamma_0^2 G(T), \quad (2)$$

where  $\gamma_0$  is the critical shear strain leading to the instability of local shearing events,  $G(T)$  is the shear modulus at temperature  $T$ . Zink et al. have found that the critical strain of metallic glasses during shear deformation are almost the same at various temperatures ( $T < T_g$ ) [35]. So in the following section, the critical shear strain  $\gamma_0$  is considered to be independent of temperature. The increase of internal energy can be expressed as

$$Q = \rho V_s \int_0^T C_p(T) dT, \quad (3)$$

where  $\rho$  is the density of BMGs,  $C_p(T)$  is the specific heat capacity at constant pressure. For metallic glasses materials between 0 K and  $T_g$ , the linear thermal expansion coefficient  $\alpha$  is negligible ( $10^{-5}$ ). Thus,  $V_s$  and  $\rho$  are considered not to change with temperature. Substituting  $T = 0$  K into Eq. (1), we obtain

$$E_{\text{cri}} = \gamma_0^2 G(0), \quad (4)$$

By plugging  $T = T_g$  into Eq. (1), we have

$$E_{\text{cri}} = \gamma_0^2 G(T_g) + \kappa \rho \int_0^{T_g} C_p(T) dT. \quad (5)$$

Incorporating Eqs. (4) and (5), we get

$$\kappa = \frac{\gamma_0^2 [G(0) - G(T_g)]}{\rho \int_0^{T_g} C_p(T) dT}. \quad (6)$$

Incorporating Eqs. (1)–(4) and (6), we can obtain

$$G(T) = G(0) - \frac{\int_0^T C_p(T) dT}{\int_0^{T_g} C_p(T) dT} [G(0) - G(T_g)]. \quad (7)$$

Varshni proposed that shear modulus  $G$  is reduced to a fixed value at the melting point, i.e.,  $G(T_m) = f_m G(0)$ , where  $f_m$  should be the same for substances with similar structure and binding [12]. Because there are many places in common between the melting point and the glass transition temperature, the glass transition can be assumed to occur when the shear modulus  $G$  is reduced to a fixed value, i.e.,  $G(T_g) = f_g G(0)$  [36]. Lu et al. compared the shear moduli of 47 BMGs at 0 K with those at glass transition temperatures [ $G(T_g)$ ], obtained that the ratios [ $f_g$ ] of  $G(T_g)/G(0)$  are almost the same and have a value around 0.85 [22]. Then, Eq. (7) can be simplified as

$$G(T) = G(0) \left[ 1 - \frac{\int_0^T C_p(T) dT}{\int_0^{T_g} C_p(T) dT} (1 - f_g) \right] \\ \approx G(0) \left[ 1 - 0.15 \frac{\int_0^T C_p(T) dT}{\int_0^{T_g} C_p(T) dT} \right]. \quad (8)$$

The specific heat capacity at constant pressure  $C_p(T)$  is defined as:

$$C_p(T) = [C_v(T) + 2\alpha^2 VBT]/M, \quad (9)$$

where  $C_v(T)$  is the heat capacity at a constant volume,  $V$  is the molar volume,  $B$  is the bulk modulus,  $M$  is the molar mass and  $\alpha$  is the linear thermal expansion coefficient. And  $C_v(T)$  can be obtained by the Debye model as follow:

$$C_v(T) = 9Nk_B \left( \frac{T}{\theta_D} \right)^3 \int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x - 1)^2} dx, \quad (10)$$

where  $N$  is the Avogadro number,  $k_B$  is the Boltzmann constant, and  $\theta_D$  is the Debye temperature. To ignore the high order small quantity  $\alpha^2$ , we have

$$C_p(T) = \frac{9Nk_B}{M} \left( \frac{T}{\theta_D} \right)^3 \int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x - 1)^2} dx. \quad (11)$$

By plugging Eq. (11) into Eq. (8), we get

$$G(T) = G(0) \left[ 1 - 0.15 \times \int_0^T \left( \frac{T}{\theta_D} \right)^3 \int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x - 1)^2} dx dT \right. \\ \left. / \int_0^{T_g} \left( \frac{T}{\theta_D} \right)^3 \int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x - 1)^2} dx dT \right]. \quad (12)$$

So the variation in shear modulus with temperature for BMGs can be predicted by Eq. (12). And the inherent relationship between the shear modulus, the Young's modulus, the glass transition temperature and the Debye temperature is revealed. The shear modulus at 0 K [ $G(0)$ ] can be obtained by substituting an arbitrary reference temperature in Eq. (12) which can be expressed by the specific length scale  $\lambda$  based on Wu's work [20]. The Debye temperature of BMGs [ $\theta_D$ ] can be obtained from the room temperature elastic moduli [37],

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